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Uploading C:\Program Files\Stnexp\Queries\10529634-Full-Final.str

L1 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 16:47:57 ON 03 JAN 2008

L1 STRUCTURE UPLOADED

L2 62 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:48:46 ON 03 JAN 2008

L3 20 S L2

L4 1 S US200!-529634/APPS

L5 19 S L3 NOT L4

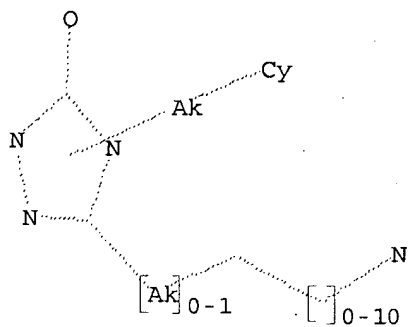
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SAV TEM L2 BRD529634/APPS BRD529634/A

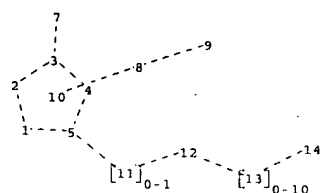
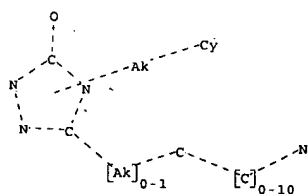
=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.



chain nodes :

7 8 9 11

ring nodes :

1 2 3 4 5

ring/chain nodes :

12 13 14

chain bonds :

3-7 5-11 8-9 11-12

ring/chain bonds :

12-13 13-14

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-7 4-5 5-11 8-9 11-12 12-13 13-14

isolated ring systems :

containing 1 :

Match level :

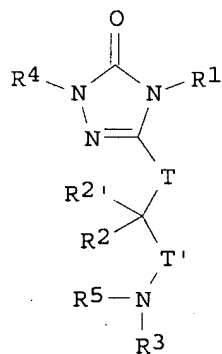
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS

Generic attributes :

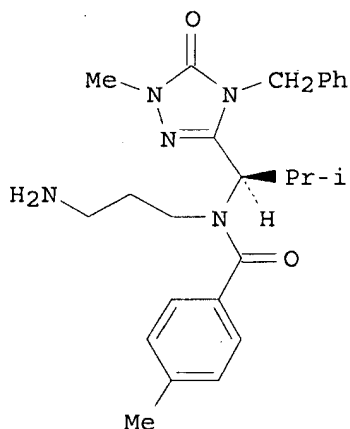
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Saturation : Unsaturated

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2004:331911 CAPLUS
 DN 140:339330
 TI Preparation of 1,2,4-triazole-5-ones as inhibitors of mitotic kinesin KSP
 IN Bergnes, Gustave; Qian, Xianping; Morgans, David J., Jr.; Knight, Steven
 David; Dhanak, Dashyant
 PA Cytokinetics, Inc., USA; Smithkline Beecham Corporation
 SO PCT Int. Appl., 89 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004032840	A2	20040422	WO 2003-US31413	20031002
	WO 2004032840	A3	20041014		
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	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
	LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,				
	PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,				
	TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,				
	KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,				
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	BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2501938	A1	20040422	CA 2003-2501938	20031002
	AU 2003282665	A1	20040504	AU 2003-282665	20031002
	EP 1558588	A2	20050803	EP 2003-774548	20031002
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	BR 2003015247	A	20050830	BR 2003-15247	20031002
	JP 2006502219	T	20060119	JP 2004-543136	20031002
	CN 1726198	A	20060125	CN 2003-80105737	20031002
	NZ 539643	A	20061130	NZ 2003-539643	20031002
	MX 2005PA03830	A	20050623	MX 2005-PA3830	20050411
	NO 2005002267	A	20050531	NO 2005-2267	20050510
	ZA 2005003733	A	20060222	ZA 2005-3733	20050510
	US 2006189671	A1	20060824	US 2005-529634	20051116 <--
PRAI	US 2002-417889P	P	20021011		
	WO 2003-US31413	W	20031002		
OS	MARPAT 140:339330				
GI					



I



II

AB Title compds. I [T, T' = bond, alkylene; R1 = H, alkyl, aryl, etc.; R2-2' = H, alkyl, aryl, etc.; R3 = H, alkyl, aryl, etc.; R4 = H, alkyl, carboxyalkyl, etc.; R5 = H, alkyl, aryl, etc.] are prepared For instance, (R)-N-(3-aminopropyl)-N-[1-(4-benzyl-1-methyl-5-oxo-4,5-dihydro-1H-[1,2,4]triazol-3-yl)-2-methylpropyl]-4-methylbenzamide (II) is prepared in 9 steps from Cbz-D-valine. I are useful for treating cellular proliferative diseases and disorders by modulating the activity of KSP.

L5 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:1278448 CAPLUS Full-text

DN 147:502353

TI Fused pyrazole derivatives as cardiovascular agents, their preparation, pharmaceutical compositions, and use in therapy

IN Schirok, Hartmut; Griebenow, Nils; Fuerstner, Chantal; Mittendorf, Joachim; Stasch, Johannes-Peter; Munder, Frank; Schlemmer, Karl-Heinz; Heitmeier, Stefan; Stoll, Friederike

FA Bayer HealthCare AG, Germany

SO PCT Int. Appl., 12pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007124854	A1	20071108	WO 2007-EP3342	20070417
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102060620327	A1	20071127	DE 2006-102006020327	20060427
PRAI DE 2006-102006020327	A	20060427		
OS MARPAT 147:502353				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to fused pyrazole derivs. of general formula I, which are active as cardiovascular agents. In compds. I, R1 is (un)substituted Ph, (un)substituted pyridinyl, (un)substituted furyl, (un)substituted thienyl, (un)substituted thiazolyl, (un)substituted oxazolyl, (un)substituted isothiazolyl, or (un)substituted isoxazolyl; R2 is oxadiazolinone, oxadiazolinethione, thiadiazolinone, (un)substituted triazolinone, or (un)substituted imidazolinone; X is CH, C(R3), or N; Y is CH, C(R3), or N, provided that Y is N only if X is also N; n is 0, 1, or 2; and each R3 is independently selected from halo, cyano, C1-4 alkyl, trifluoromethyl, amino, C1-4 alkoxy, and trifluoromethoxy, including salts, solvates, and solvates of salts thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I together with a pharmaceutically acceptable adjuvant, optionally in combination with an addnl. active agent, as well as to the use of the compns. for the treatment of cardiovascular diseases. Heterocyclization of 2-fluoropyridine with Et trifluoroacetate and hydrazine hydrate followed by condensation with ammonia and substitution of 2-fluorobenzyl bromide resulted in the formation of pyrazolopyridine II, which underwent addition of hydroxylamine hydrochloride, condensation with N,N'-thiocarbonyldiimidazole, and rearrangement to give

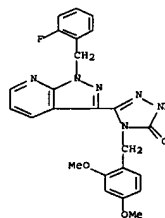
thiadiazolinone III. The compds. of the invention were found to express vasorelaxant activity, e.g., compound III expressed an IC50 value of 0.45 µM.

IT 956010-91-6P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-3H-1,2,4-triazol-3-one 956010-92-7P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one 956010-93-8P, 4-[(2,4-dimethoxybenzyl)methyl]-2-ethyl-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-02-2P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-propyl-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-03-3P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-isobutyl-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-04-4P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-isopropyl-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-05-5P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-(2-fluoroethyl)-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-06-6P, 2-[(2,2-difluoroethyl)-4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-07-7P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-(2,2,2-trifluoroethyl)-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-08-8P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-(2-hydroxyethyl)-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-09-9P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-10-2P, 4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-(3-morpholin-4-yl)propyl-2,4-dihydro-3H-1,2,4-triazol-3-one 956011-11-3P, 3-[4-[(2,4-dimethoxybenzyl)methyl]-5-[1-[(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-2-oxo-4,5-dihydro-1H-1,2,4-triazol-1-yl]propanenitrile

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

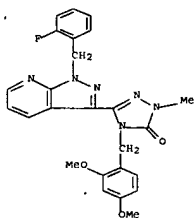
(intermediate; preparation of fused pyrazole derivs. as cardiovascular agents)

RN 956010-91-6 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro- (CA INDEX NAME)



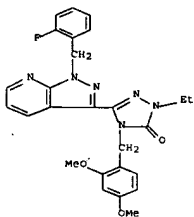
RN 956010-92-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-methyl- (CA INDEX NAME)



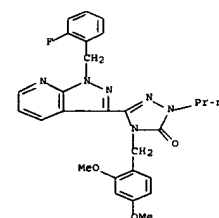
RN 956010-93-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-2-ethyl-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro- (CA INDEX NAME)



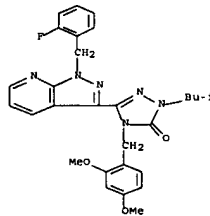
RN 956011-02-2 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-propyl- (CA INDEX NAME)



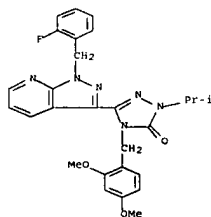
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CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-(2-methylpropyl)- (CA INDEX NAME)



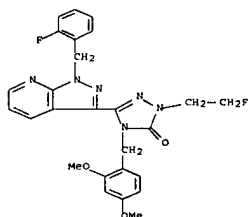
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CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-(1-methylethyl)- (CA INDEX NAME)



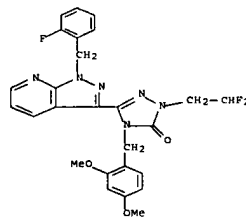
RN 956011-05-5 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-2-[(2-fluorophenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro- (CA INDEX NAME)



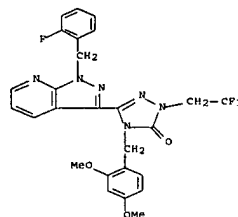
RN 956011-06-6 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(2,2-difluoroethyl)-4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro- (CA INDEX NAME)



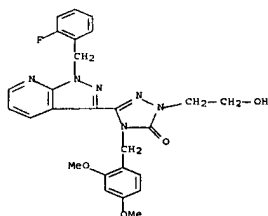
RN 956011-07-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-[(2,2,2-trifluoroethyl)- (CA INDEX NAME)



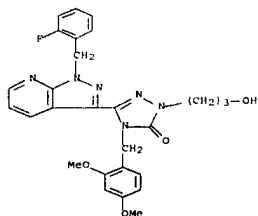
RN 956011-08-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-[(2-hydroxyethyl)- (CA INDEX NAME)



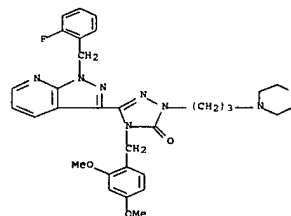
RN 956011-09-9 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-[(3-hydroxypropyl)- (CA INDEX NAME)



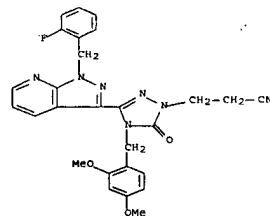
RN 956011-10-2 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[(2,4-dimethoxyphenyl)methyl]-5-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-2,4-dihydro-2-[(3-morpholinyl)propyl]- (CA INDEX NAME)



RN 956011-11-3 CAPLUS

CN 1H-1,2,4-Triazole-1-propanenitrile, 4-[(2,4-dimethoxyphenyl)methyl]-3-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-4,5-dihydro-5-oxo- (CA INDEX NAME)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2006:655929 CAPLUS [Full-text](#)
 DN 145:124562
 TI Preparation of pyrazole derivatives that modulate the activity of CDK, GSK and aurora kinases
 IN Berdini, Valerio; O'Brien, Michael Alistair; Carr, Maria Grazia; Davies, Nicholas Gareth; Morse, Gill; Adrian Liam; Navarro, Eva Figueroa; Howard, Steven; Trewartha, Gary; Woodhead, Andrew James; Woolford, Alison Jo-Anne; Wyatt, Paul Graham
 PA Astex Therapeutics Limited, UK
 SO PCT Int. Appl., 200 pp.

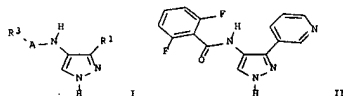
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006070198	A1	20060706	WO 2005-GB5102	20051230
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, ID, IL, IN, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1836188	A1	20070926	EP 2005-823522	20051230
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PRA1 GB 2004-28528	A	20041230		
US 2004-640474P	P	20041230		
WO 2005-GB5102	W	20051230		
OS MARPAT 145:124562				
GI				



AB Title compds. I [R1 = (un)substituted heterocyclic group having at least one atom selected from N, O or S; R2 = H, halo, alkoxy, etc.; R3 = (un)substituted carbocycle and heterocycle or hydrocarbyl group; A = bond or Y(B)n; Y = bond or alkylene chain of 1-3 carbon atoms in length; B = CO, NHCO, OCO, etc.; n = 0 or 1, and their salts or tautomers or N-oxides or solvates thereof, are prepared and disclosed as modulators of CDK, GSK and aurora kinases. Thus, e.g., II was prepared by cyclocondensation of 3-dimethylamino-1-pyridin-3-ylpropanone with hydrazine to form the pyrazole moiety which was nitrated, reduced, and amidated with 2,6-difluorobenzoic acid. Compds. of the invention were assayed against CDK1 and CDK2, e.g., II demonstrated IC50 values of less than 1µM against CDK1 and CDK2 activity. Addnl. bioassays were described.

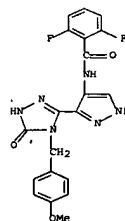
IT 896467-76-4P, 2,6-Difluoro-N-[3-[(4-methoxybenzyl)-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]-1H-pyrazol-4-yl]benzamide
 896467-72-4P 896467-72-5P 896467-75-8P
 896467-79-0P 896467-79-1P 896467-80-4P
 896467-83-7P 896467-84-8P 896467-85-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of pyrazole derivs. that modulate the activity of CDK, GSK and aurora kinases)

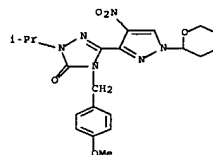
RN 896467-56-4 CAPLUS

CN Benzamide, N-[3-[(4,5-dihydro-4-[(4-methoxyphenyl)methyl]-5-oxo-1H-1,2,4-triazol-3-yl)-1H-pyrazol-4-yl]-2,6-difluoro- (CA INDEX NAME)



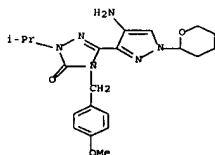
RN 896467-72-4 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-[(4-methoxyphenyl)methyl]-2-(1-methylethyl)-5-(4-nitro-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazol-3-yl)- (CA INDEX NAME)



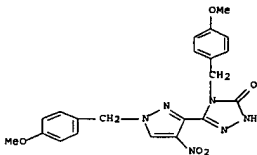
RN 896467-73-5 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-[4-amino-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazol-3-yl]-2,4-dihydro-4-[(4-methoxyphenyl)methyl]-2-(1-methylethyl)- (CA INDEX NAME)



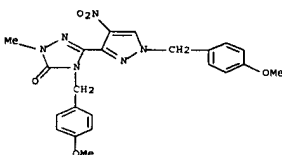
RN 896467-76-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-[(4-methoxyphenyl)methyl]-5-[1-[(4-methoxyphenyl)methyl]-4-nitro-1H-pyrazol-3-yl]-2-methyl- (CA INDEX NAME)



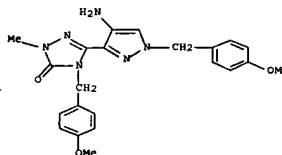
RN 896467-78-0 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-[(4-methoxyphenyl)methyl]-5-[1-[(4-methoxyphenyl)methyl]-4-nitro-1H-pyrazol-3-yl]-2-methyl- (CA INDEX NAME)



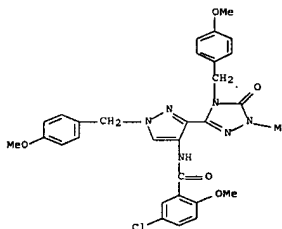
RN 896467-79-1 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-[4-amino-1-[(4-methoxyphenyl)methyl]-1H-pyrazol-3-yl]-2,4-dihydro-4-[(4-methoxyphenyl)methyl]-2-methyl- (CA INDEX NAME)



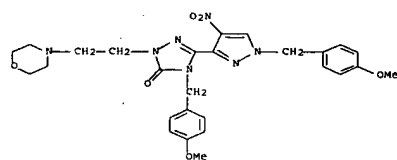
RN 896467-80-4 CAPLUS

CN Benzamide, 5-chloro-N-[3-[(4,5-dihydro-4-[(4-methoxyphenyl)methyl]-1-methyl-5-oxo-1H-1,2,4-triazol-3-yl)-1-[(4-methoxyphenyl)methyl]-1H-pyrazol-4-yl]-2-methoxy- (CA INDEX NAME)



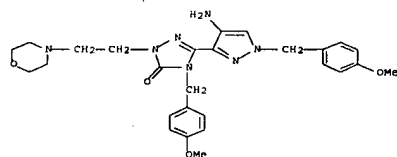
RN 896467-83-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-[(4-methoxyphenyl)methyl]-5-[1-[(4-methoxyphenyl)methyl]-4-nitro-1H-pyrazol-3-yl]-2-[2-(4-morpholinylethyl)- (CA INDEX NAME)



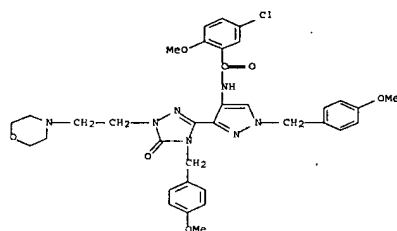
RN 896467-84-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-[4-amino-1-[(4-methoxyphenyl)methyl]-1H-pyrazol-3-yl]-2,4-dihydro-4-[(4-methoxyphenyl)methyl]-2-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)



RN 896467-85-9 CAPLUS

CN Benzamide, 5-chloro-N-[3-[4,5-dihydro-4-[(4-methoxyphenyl)methyl]-1-[2-(4-morpholinyl)ethyl]-5-oxo-1H-1,2,4-triazol-3-yl]-1-[(4-methoxyphenyl)methyl]-1H-pyrazol-4-yl]-2-methoxy- (CA INDEX NAME)



AB Title compds. [1; whereby the residue NHC(Y)NHR2 is bonded to the aromatic in the position 2, 3, 5, or 6; X = NR6, CR1R4; Y = O, S; R2 = cycloalkyl, (substituted) aryl; R3 = H, (substituted) alkyl; R5 = H, halo, OH, alkoxy, amino, alkylamino, alkyl; R1 = (substituted) alkyl, aryl; R4 = (substituted) alkyl, aryl; or R1R4 = (substituted) cycloalkyl; R6 = aryl, (substituted) cycloalkyl, alkyl], were prepared. Thus, 4-chloro-3-fluorophenyl isocyanate was treated with a solution of 5-(3-aminophenyl)-4,4-dimethyl-2,4-dihydro-3H-pyrazol-3-one (preparation given) in AcOEt and THF followed by stirring over night at room temperature to give 90% N-(3-chloro-4-fluorophenyl)-N'-(3-(4,4-dimethyl-5-oxo-4,5-dihydro-1H-pyrazol-3-yl)phenyl)urea. The latter inhibited human cytomegalovirus (HCMV) with EC50 = 0.4 μM.

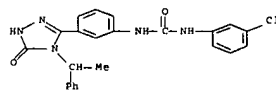
IT 569345-77-3P 569345-78-4P 569345-79-5P 569345-80-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (pyrazolylphenyl)ureas and (triazolylphenyl)ureas as antiviral agents for treatment of cytomegalovirus)

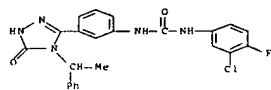
RN 569345-77-3 CAPLUS

CN Urea, N-(3-chlorophenyl)-N'-(3-[4,5-dihydro-5-oxo-4-(1-phenylethyl)-1H-1,2,4-triazol-3-yl]phenyl)- (CA INDEX NAME)



RN 569345-78-4 CAPLUS

CN Urea, N-(3-chloro-4-fluorophenyl)-N'-(3-[4,5-dihydro-5-oxo-4-(1-phenylethyl)-1H-1,2,4-triazol-3-yl]phenyl)- (CA INDEX NAME)



RN 569345-79-5 CAPLUS

CN Urea, N-(4-chloro-2-methylphenyl)-N'-(3-[4,5-dihydro-5-oxo-4-(1-phenylethyl)-1H-1,2,4-triazol-3-yl]phenyl)- (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

LS ANSWER 3 OF 19 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 2003:589439 CAPLUS Full-text

DN 139:133572

TI Preparation of (pyrazolylphenyl)ureas and (triazolylphenyl)ureas as antiviral agents for the treatment of cytomegalovirus

IN Munberg, Tobias; Betz, Ulrich; Kleymann, Gerald; Nikolic, Susanne; Reefsclaeger, Juergen; Schohe-Loop, Rudolf; Zimmermann, Holger; Zumpe, Franz; Bender, Wolfgang; Henninger, Kerstin; Hewlett, Guy; Jensen, Axel; Keldenich, Joerg

PA Bayer AG, Germany

SO Ger. Offen., 32 pp.

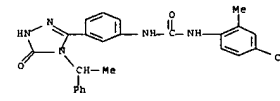
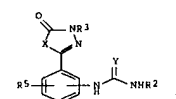
CODEN: GWXXBX

DT Patent

LA German

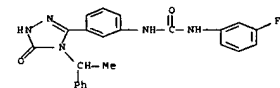
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10203086	A1	20030731	DE 2002-10203086	20020128
CA 2474456	A1	20030807	CA 2003-2474456	20030116
WO 2003064394	A1	20030807	WO 2003-EP376	20030116
WO 2003064394	A8	20031224		
M: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
EP 1472229	A1	20041103	EP 2003-734671	20030116
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005521669	T	20050721	JP 2003-564017	20030116
PRAI DE 2002-10203086	A	20020128		
WO 2003-EP376	W	20030116		
OS MARPAT 139:133572				
GI				



RN 569345-80-8 CAPLUS

CN Urea, N-(3-[4,5-dihydro-5-oxo-4-(1-phenylethyl)-1H-1,2,4-triazol-3-yl]phenyl)-N'-(3-fluorophenyl)- (CA INDEX NAME)



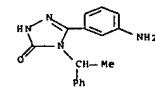
IT 569345-57-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (pyrazolylphenyl)ureas and (triazolylphenyl)ureas as antiviral agents for treatment of cytomegalovirus)

RN 569345-57-9 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-(3-aminophenyl)-2,4-dihydro-4-(1-phenylethyl)- (CA INDEX NAME)



LS ANSWER 4 OF 19 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 2003:277532 CAPLUS Full-text

DN 139:117370

TI Cyclization of semicarbazide derivatives of 3-methyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazole-4-acetic acid

AU Dobosz, Maria; Pitucha, Monika; Dybala, Izabela; Kozioł, Anna E.

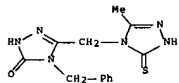
CS Department of Organic Chemistry, Faculty of Pharmacy, Medical University, Lublin, 20-081, Pol.

SO Collection of Czechoslovak Chemical Communications (2003), 68(4), 792-800

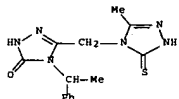
CODEN: CCCCAK; ISSN: 0010-0765

PB Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

DT Journal
LA English
OS CASREACT 139:117370
AB By the reaction of hydrazide of 3-methyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazole-4-acetic acid (1) with isocyanates, 3-methyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazole-4-acetosemicarbazide derivs. 2 were obtained. Cyclization of these compds. in the presence of 2% NaOH led to the formation of 4,5-dihydro-1H-1,2,4-triazol-5-one derivs. 3, which was confirmed by X-ray anal. of 3b.
IT 561013-99-8P 561014-03-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclization of semicarbazide derivs. of methylthioxodihydrotriazole acetic acid)
RN 561013-99-8 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[(1,5-dihydro-3-methyl-5-thioxo-4H-1,2,4-triazol-4-yl)methyl]-2,4-dihydro-4-(phenylethyl)- (CA INDEX NAME)



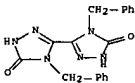
RN 561014-03-7 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[(1,5-dihydro-3-methyl-5-thioxo-4H-1,2,4-triazol-4-yl)methyl]-2,4-dihydro-4-(1-phenylethyl)- (CA INDEX NAME)



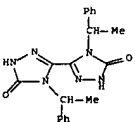
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:123960 CAPLUS Full-text
DN 139:85282
TI The reactions of cyclization of semicarbazide derivatives of 1,3-diphenyl-1,2,4-triazolin-5-thione-4-acetic acid
AU Dobosz, Maria; Pitucha, Monika; Chudnicka, Alina
CS Department of Organic Chemistry, Faculty of Pharmacy, Medical University, Lublin, 20-081, Pol.
SO Acta Polonicae Pharmaceutica (2002), 59(5), 371-377
CODEN: APHAX; ISSN: 0001-6837
PB Polish Pharmaceutical Society
DT Journal

CS Department of Organic Chemistry, Faculty of Pharmacy, Medical University, Lublin, 20-081, Pol.
SO Acta Polonicae Pharmaceutica (2001), 58(4), 307-311
CODEN: APHAX; ISSN: 0001-6837
PB Polish Pharmaceutical Society
DT Journal
LA English
OS CASREACT 137:125122
AB In the reaction of oxalic acid hydrazide with isocyanates, new derivs. RHNCONHNHCOCONHNHCONHR [R = (un)substituted Ph, cyclohexyl, etc.] of semicarbazide were obtained. Cyclization of these derivs. with an aqueous 2% sodium hydroxide led to formation of new derivs. of Δ2-1,2,4-triazolin-5-one.
IT 444327-48-4P 444327-49-5P 444327-52-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of triazolinones by cyclization of acylated oxalic acid semicarbazides)
RN 444327-48-4 CAPLUS
CN [3,3'-Bi-1H-1,2,4-triazole]-5,5'-(4H,4'H)-dione, 4,4'-bis(phenylethyl)- (9CI) (CA INDEX NAME)

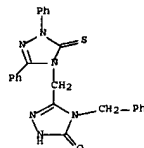


RN 444327-49-5 CAPLUS
CN [3,3'-Bi-1H-1,2,4-triazole]-5,5'-(4H,4'H)-dione, 4,4'-bis(1-phenylethyl)- (9CI) (CA INDEX NAME)

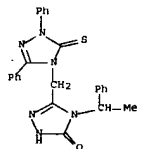


RN 444327-52-0 CAPLUS
CN [3,3'-Bi-1H-1,2,4-triazole]-5,5'-(4H,4'H)-dione, 4,4'-dibenzoyl- (9CI) (CA INDEX NAME)

LA English
OS CASREACT 139:85282
AB In the reaction of hydrazide of 1,3-diphenyl-1,2,4-triazolin-5-thione-4-acetic acid with isocyanates, semicarbazide derivs. of 1,3-diphenyl-1,2,4-triazolin-5-thione-4-acetic acid [I-X] were obtained. Cyclization of these compds. in the presence of 2% NaOH led to the formation of derivs. of 1,2,4-triazolin-5-one [XI-XX].
IT 553653-84-2P 553653-86-4P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(cyclization of semicarbazide derivs. of 1,3-diphenyl-1,2,4-triazolin-5-thione-4-acetic acid)
RN 553653-84-2 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[(1,5-dihydro-1,3-diphenyl-5-thioxo-4H-1,2,4-triazol-4-yl)methyl]-2,4-dihydro-4-(phenylethyl)- (CA INDEX NAME)

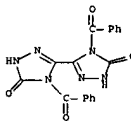


RN 553653-86-4 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[(1,5-dihydro-1,3-diphenyl-5-thioxo-4H-1,2,4-triazol-4-yl)methyl]-2,4-dihydro-4-(1-phenylethyl)- (CA INDEX NAME)



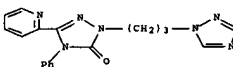
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:835243 CAPLUS Full-text
DN 137:125122
TI Synthesis of new derivatives of bis-3-(4-R-Δ2-1,2,4-triazolin-5-one)
AU Pachuta-Stec, Anna; Dobosz, Maria

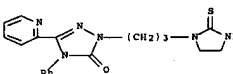


RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:567877 CAPLUS Full-text
DN 129:220612
TI Synthesis of 1-(3-aminopropyl)-1,2,4-triazolin-5-one derivatives
AU Maliszewska-Guz, Alicja; Dobosz, Maria
CS Department of Organic Chemistry, School of Medicine, Lublin, 20-081, Pol.
SO Acta Polonicae Pharmaceutica (1997), 54(2), 141-145
CODEN: APHAX; ISSN: 0001-6837
PB Polish Pharmaceutical Society
DT Journal
LA English
AB The reaction of 4-phenyl-3-(2-pyridyl)-1,2,4-triazolin-5-one with 1-bromo-3-chloropropane gives the 1-(3-chloropropyl) derivative which reacted with secondary amines or with ethylenediamine to give the aminopropyl analogs. The ethylenediamine derivative was cyclized with CS2 to give the imidazopyrrol derivative
IT 195139-69-6P 195139-72-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminopropyltriazolinone derivs.)
RN 195139-69-6 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-phenyl-5-(2-pyridinyl)-2-[3-(1H-1,2,4-triazol-1-yl)propyl]- (CA INDEX NAME)



RN 195139-72-1 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-phenyl-5-(2-pyridinyl)-2-[3-(2-thioxo-1-imidazolidinyl)propyl]- (CA INDEX NAME)



L5 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 1997:16548 CAPLUS [Full-text](#)

DN 126:152804

TI Spirolactone or other epoxy-free spirolactone-type aldosterone receptor antagonist in combination with angiotensin II antagonist for treatment of circulatory and cardiovascular disorders, including congestive heart failure

IN MacLaughlin, Todd E.; Schuh, Joseph R.

PA G.D. Searle and Co., USA; MacLaughlin, Todd E.; Schuh, Joseph R.

PCT Int. Appl., 210 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640258	A2	19961219	WO 1996-US9342	19960605
WO 9640258	A3	19970123		
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
CA 2224222	A1	19961219	CA 1996-2224222	19960605
AU 9661580	A	19961230	AU 1996-61580	19960605
EP 831911	A2	19980401	EP 1996-919173	19960605
R: AT, BE, CH, DE, DK, ES, FR, GB, GM, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1192696	A	19980909	CN 1996-196086	19960605
BR 9604505	A	19990706	BR 1996-8505	19960605
JP 11509938	T	19990831	JP 1997-501683	19960605
AT 216261	T	20020515	AT 1996-919173	19960605
PT 831911	T	20020930	PT 1996-919173	19960605
ES 2175094	T3	20021116	ES 1996-919173	19960605
CZ 291268	B6	20030115	CZ 1997-3848	19960605
IL 122246	A	20040601	IL 1996-122246	19960605
US 2004102423	A1	20040527	US 2002-271362	20021015
AU 2003204258	A1	20030619	AU 2003-204258	20030519
PRAT 1995-486089	A	19950607		
WO 1996-US9342	A	19960605		
US 1996-773383	B1	19961226		
US 1997-977409	B1	19971124		
US 1999-415043	B1	19991007		
AU 2000-42642	A3	20000623		

OS MARPAT 126:152804

AB A combination therapy is disclosed which comprises a therapeutically-effective amount of an epoxy-free spirolactone-type aldosterone receptor antagonist and a therapeutically-effective amount of an angiotensin II receptor antagonist for treatment of circulatory disorders, including cardiovascular disorders, e.g. hypertension and congestive heart failure. Preferred angiotensin II receptor antagonists are those compds. having high potency and bioavailability and which are characterized in having an imidazole or triazole moiety attached to a biphenylmethyl or pyridinyl/phenylmethyl moiety. A preferred epoxy-free spirolactone-type aldosterone receptor antagonist is spironolactone. A preferred combination therapy includes the angiotensin II receptor antagonist 5-[2-[5-[(3,5-dibutyl-1H-1,2,4-triazol-1-

JP 11507627	T	19990706	JP 1996-501678	19960605
NZ 310730	A	20010126	NZ 1996-310730	19960605
RU 2166330	C2	20010510	RU 1998-100250	19960605
IL 122242	A	20010724	IL 1996-122242	19960605
AT 209047	T	20011215	AT 1996-919170	19960605
ES 2167571	T3	20020516	ES 1996-919170	19960605
PT 831910	T	20020531	PT 1996-919170	19960605
RO 118046	B1	20030130	RO 1997-2272	19960605
PL 185150	B1	20030331	PL 1996-324001	19960605
CN 1522701	A	20040825	CN 2004-10002796	19960605
CZ 297475	B6	20070509	CZ 1997-3850	19960605
US 6653306	B1	20031125	US 1997-781786	19970109
NO 9705741	A	19980129	NO 1997-5741	19971205
NO 318184	B1	20050214		
AU 2003202486	A1	20030612	AU 2003-202486	20030326
PRAT 1995-486456	A	19950607		
WO 1996-US9335	W	19960605		
AU 2000-53494	A3	20000818		

OS MARPAT 126:152803

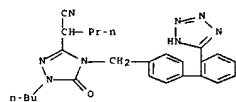
AB A combination therapy comprising a therapeutically-effective amount of an epoxy-steroidal aldosterone receptor antagonist and a therapeutically-effective amount of an angiotensin II receptor antagonist is described for treatment of circulatory disorders, including cardiovascular disorders, e.g. hypertension and congestive heart failure. Preferred angiotensin II receptor antagonists are those compds. having high potency and bioavailability and which are characterized in having an imidazole or triazole moiety attached to a biphenylmethyl or pyridinyl/phenylmethyl moiety. Preferred epoxy-steroidal aldosterone receptor antagonists are 20-11a-substituted epoxy moieties. A preferred combination therapy includes the angiotensin II receptor antagonist 5-[2-[5-[(3,5-dibutyl-1H-1,2,4-triazol-1-yl)methyl]-2-pyridinyl]phenyl]-1H-tetrazole and the aldosterone receptor antagonist epoxyexrenone.

IT 139476-43-0

RI: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (epoxy-steroidal aldosterone antagonist and angiotensin II antagonist combination therapy for treatment of cardiovascular disorders, including congestive heart failure)

RN 139476-43-0 CAPLUS

CN 1H-1,2,4-Triazole-3-acetonitrile, 1-butyl-4,5-dihydro-5-oxo-u-propyl-4-[(2'-[(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)



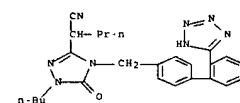
yl)methyl]-2-pyridinyl]phenyl]-1H-tetrazole and the aldosterone receptor antagonist spironolactone.

IT 139476-43-0

RI: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (spironolactone or other epoxy-free spirolactone-type aldosterone receptor antagonist in combination with angiotensin II antagonist for treatment of circulatory and cardiovascular disorders, including congestive heart failure)

RN 139476-43-0 CAPLUS

CN 1H-1,2,4-Triazole-3-acetonitrile, 1-butyl-4,5-dihydro-5-oxo-u-propyl-4-[(2'-[(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 1997:168547 CAPLUS [Full-text](#)

DN 126:152803

TI Epoxy-steroidal aldosterone antagonist and angiotensin II antagonist combination therapy for treatment of cardiovascular disorders, including congestive heart failure

IN Alexander, John C.; Schuh, Joseph R.; Gorczynski, Richard J.

PA G.D. Searle and Co., USA; Alexander, John C.; Schuh, Joseph R.; Gorczynski, Richard J.

PCT Int. Appl., 218 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640257	A1	19961219	WO 1996-US9335	19960605
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
CA 2224079	A1	19961219	CA 1996-2224079	19960605
AU 9661577	A	19961230	AU 1996-61577	19960605
AU 725689	B2	20001019		
EP 831910	A1	19980401	EP 1996-919170	19960605
EP 831910	B1	20011121		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1192697	A	19980909	CN 1996-196155	19960605
BR 9609066	A	19990126	BR 1996-9066	19960605

DN 126:152800

TI Method to treat cardiofibrosis or cardiac hypertrophy with a combination of an angiotensin II antagonist and spironolactone or other epoxy-free spirolactone-type aldosterone receptor antagonist

IN McMahon, Ellen G.; Olins, Gillian M.; Schuh, Joseph R.

PA G.D. Searle and Co., USA; McMahon, Ellen G.; Olins, Gillian M.; Schuh, Joseph R.

PCT Int. Appl., 208 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640256	A1	19961219	WO 1996-US8823	19960605
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
AU 9659822	A	19961230	AU 1996-59822	19960605
US 2004067915	A1	20040408	US 2003-429410	20030505
PRAT 1995-485935	A	19950607		
WO 1996-US8823	W	19960605		
US 1997-908584	B1	19970808		
US 1999-439309	B1	19991112		

OS MARPAT 126:152800

AB A therapeutic method is described for treating cardiofibrosis or cardiac hypertrophy using a combination therapy comprising a therapeutically-effective amount of an epoxy-free spirolactone-type aldosterone receptor antagonist and a therapeutically-effective amount of an angiotensin II receptor antagonist. Preferred angiotensin II receptor antagonists are those compds. having high potency and bioavailability and which are characterized in having an imidazole or triazole moiety attached to a biphenylmethyl or pyridinyl/phenylmethyl moiety. A preferred epoxy-free spirolactone-type aldosterone receptor antagonist is spironolactone. A preferred combination therapy includes the angiotensin II receptor antagonist 5-[2-[5-[(3,5-dibutyl-1H-1,2,4-triazol-1-yl)methyl]-2-pyridinyl]phenyl]-1H-tetrazole and the aldosterone receptor antagonist spironolactone.

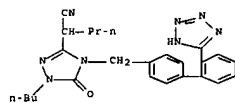
IT 139476-43-0

RI: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(angiotensin II antagonist combination with spironolactone or other epoxy-free spirolactone-type aldosterone receptor antagonist for treatment of cardiofibrosis or cardiac hypertrophy)

RN 139476-43-0 CAPLUS

CN 1H-1,2,4-Triazole-3-acetonitrile, 1-butyl-4,5-dihydro-5-oxo-u-propyl-4-[(2'-[(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1997:140243 CAPLUS [Full-text](#)

DN 126:139886

TI Method to treat cardiobfibrosis or cardiac hypertrophy with a combination therapy of an angiotensin II antagonist and an epoxy-steroidal aldosterone antagonist

IN Egan, James J.; McMahon, Ellen G.; Olins, Gillian M.; Schuh, Joseph R.
PA G.D. Searle and Co., USA; Egan, James J.; McMahon, Ellen G.; Olins, Gillian M.; Schuh, Joseph R.

SO PCT Int. Appl., 202 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640255	A2	19961219	WO 1996-US8709	19960605
WO 9640255	A3	19970123		
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CP, CG, CI, CM, GA				
AU 960392	A	19961230	AU 1996-60392	19960605
US 1995-486085	A	19950607		
US 1996-US8709	W	19960605		

AB A therapeutic method is described for treating cardiobfibrosis or cardiac hypertrophy using a combination therapy comprising a therapeutically effective amount of an epoxy-steroidal aldosterone receptor antagonist and a therapeutically-effective amount of an angiotensin II receptor antagonist. Preferred angiotensin II receptor antagonists are those compds. having high potency and bioavailability and which are characterized in having an imidazole or triazole moiety attached to a biphenylmethyl or pyridinyl/phenylmethyl moiety. Preferred epoxy-steroidal aldosterone receptor antagonists are 20-spiroxane steroidal compds. characterized by the presence of a 9a,11a-substituted epoxy moiety. A preferred combination therapy includes the angiotensin II receptor antagonist 5-[2-[5-[(3,5-dibutyl-1H-1,2,4-triazol-1-yl)methyl]-2-pyridinyl]phenyl]-1H-tetrazole and the aldosterone receptor antagonist epoxymexrenone.

IT 139476-43-0

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BTOL (Biological study); PROC (Process); USES (Uses)

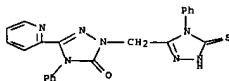
TI angiotensin II antagonist and epoxy-steroidal aldosterone antagonist combination for treatment of cardiobfibrosis or cardiac hypertrophy

RN 139476-43-0 CAPLUS

181469-95-4P 181470-00-8P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

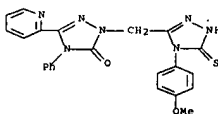
RN 181469-01-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[[4,5-dihydro-4-(4-methoxyphenyl)-5-thioxo-1H-1,2,4-triazol-3-yl)methyl]-2,4-dihydro-4-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)



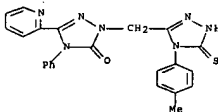
RN 181469-85-2 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[[4,5-dihydro-4-(4-methoxyphenyl)-5-thioxo-1H-1,2,4-triazol-3-yl)methyl]-2,4-dihydro-4-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)



RN 181469-90-9 CAPLUS

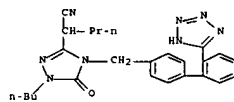
CN 3H-1,2,4-Triazol-3-one, 2-[[4,5-dihydro-4-(4-methylphenyl)-5-thioxo-1H-1,2,4-triazol-3-yl)methyl]-2,4-dihydro-4-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)



RN 181469-95-4 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[[4-(4-bromophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)methyl]-2,4-dihydro-4-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)

CN 1H-1,2,4-Triazole-3-acetonitrile, 1-butyl-4,5-dihydro-5-oxo-α-propyl-4-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:511909 CAPLUS [Full-text](#)

DN 125:221739

TI Derivatives of hydroxy-1,2,4-triazole. Part VI. Synthesis of thiosemicarbazide derivatives of the 1,2,4-triazole system

AU Dobosz, Maria; Maliszewska-Guz, Alicja

CS Zaklad Chemii Organicznej, Akad. Medycznej, Lublin, Pol.

SO Annales Universitatis Mariae Curie-Sklodowska, Sectio AA: Chemia (1995), Volume Date 1991-1992, 46-47, 51-59

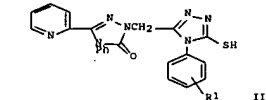
CODEN: AUMCD7; ISSN: 0137-6853

PB Uniwersytet Marii Curie-Sklodowskiej

DT Journal

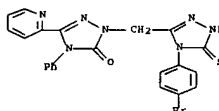
LA Polish

GI



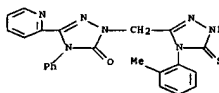
AB Triazole-containing hydrazides reacted with isothiocyanates to give thiosemicarbazides I (R = H, OMe, Me, Br) and II (R = H, 4-OMe, 4-Me, 4-Br, 2-Me). Cyclization of II gave (triazolylmethyl)triazolones (III).

IT 181469-01-8P 181469-85-2P 181469-90-9P



RN 181470-00-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[[4,5-dihydro-4-(2-methylphenyl)-5-thioxo-1H-1,2,4-triazol-3-yl)methyl]-2,4-dihydro-4-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)



L5 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:511902 CAPLUS [Full-text](#)

DN 125:221735

TI Substitution reactions of hydroxy-1,2,4-triazoles. Part II

AU Maliszewska-Guz, Alicja; Dobosz, Maria

CS Zaklad Chemii Organicznej, Akademii Medycznej, Lublin, Pol.

SO Annales Universitatis Mariae Curie-Sklodowska, Sectio AA: Chemia (1995), Volume Date 1991-1992, 46-47, 29-34

CODEN: AUMCD7; ISSN: 0137-6853

PB Uniwersytet Marii Curie-Sklodowskiej

DT Journal

LA Polish

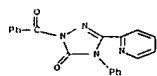
AB Reactions of 1-phenyl-3-hydroxy-1,2,4-triazole and 3-α-pyridyl-4-phenyl-5-hydroxy-1,2,4-triazole with Et chloroformate, acetic anhydride, benzoyl chloride, allyl bromide, and Et bromoacetate were studied. The reactions gave O- or N-substituted 1,2,4-triazoles.

IT 181421-84-1P

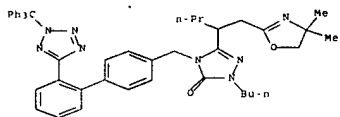
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 181421-84-1 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-benzoyl-2,4-dihydro-4-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)

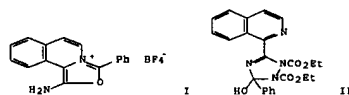


LS ANSWER 14 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1995:227811 CAPLUS Full-text
 DN 122:105706
 TI Discovery of nonpeptide, potent conformationally restricted angiotensin II receptor antagonists
 AU Huang, Horng-Chih; Chamberlain, Timothy S.; Olins, Gillian M.; Corpus, Valerie M.; Chen, Susan T.; McMahon, Ellen G.; Palomo, Maria A.; Blaine, Edward H.; Manning, Robert E.
 CS Depts. Chemistry and Cardiovascular Diseases Research, Searle R&D, St. Louis, MO, 63198, USA
 SO Bioorganic & Medicinal Chemistry Letters (1994), 4(21), 2591-6
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier
 DT Journal
 LA English
 AB A series of potent, selective, conformationally restricted angiotensin II (AII) receptor antagonists has been discovered. Two classes of conformationally restricted analogs were prepared: triazolone-based and imidazole-based biphenyl derivs. The most active compound, an imidazole-based analog, has an IC50 of 11 nM and a pA2 of 8.8.
 IT 162561 32-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of conformationally restricted angiotensin II receptor antagonists)
 RN 160561-33-1 CAPLUS
 CN 1H-1,2,4-Triazol-3-one, 2-butyl-5-[1-[(4,5-dihydro-4,4-dimethyl-2-oxazolyl)methyl]butyl]-2,4-dihydro-4-[(2'-[2-(triphenylmethyl)-2H-tetrazol-5-yl][1,1'-biphenyl]-4-yl)methyl]- (CA INDEX NAME)

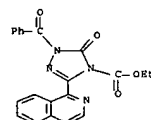


LS ANSWER 15 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1994:244873 CAPLUS Full-text
 DN 120:244873
 TI Reaction of 2-benzoyl-1,2-dihydroisoquinoline-1-carbonitrile tetrafluoroborate salt with diethyl azodicarboxylate. An unexpected

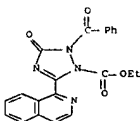
evolution of the condensation-rearrangement product
 AU Monnier, Karin; Schmitt, Gerard; Laude, Bernard; Kubicki, Marek M.; Boudot, Patrick
 CS Lab. Chim. Org., Univ. Franche-Comte, Besancon, 25030, Fr.
 SO Journal of Chemical Research, Synopses (1994), (2), 64-5,428-42
 CODEN: JKPSDC; ISSN: 0308-2342
 DT Journal
 LA English
 OS CASREACT 120:244873
 GI



AB 2-Benzoyl-1,2-dihydroisoquinoline-1-carbonitrile salt I reacted with EtO2CHNCO2Et to give the condensation-rearrangement product, triazolo-carboxylate II, in 55% yield.
 IT 154386-68-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)
 RN 154386-68-2 CAPLUS
 CN 4H-1,2,4-Triazole-4-carboxylic acid, 1-benzoyl-1,5-dihydro-3-(1-isoquinolinyl)-5-oxo-, ethyl ester (CA INDEX NAME)



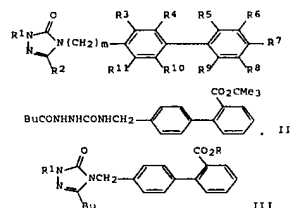
IT 154386-67-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and isomerization of)
 RN 154386-67-1 CAPLUS
 CN 1H-1,2,4-Triazole-1-carboxylic acid, 2-benzoyl-2,3-dihydro-5-(1-isoquinolinyl)-3-oxo-, ethyl ester (CA INDEX NAME)



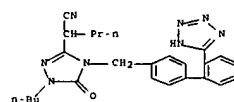
LS ANSWER 16 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1992:426573 CAPLUS Full-text
 DN 117:26573
 TI Preparation of N-substituted 1,2,4-triazolones for treatment of cardiovascular disorders
 IN Manning, Robert E.; Reitz, David B.; Huang, Horng Chih
 PA G.D. Searle and Co., USA
 SO PCT Int. Appl., 210 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9118898	A1	19911212	WO 1991-US3449	19910523
W: AT, AU, BB, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MM, NL, NO, PL, RO, SD, SE, SI, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
CA 2083735	A1	19911126	CA 1991-2083735	19910523
AU 9175030	A	19911231	AU 1991-79030	19910523
EP 531382	A1	19930317	EP 1991-910101	19910523
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05506443	T	19930922	JP 1991-509457	19910523
PRA1 US 1990-529079	A2	19900525		
WO 1991-US3449	A	19910523		

OS MARPAT 117:26573
 GI



AB 1,2,4-Triazolones [I; R1 = 2-oxo-2-(tricyclo[3.3.1.1.3,7]dec-2-yl)ethyl, 2-phenylpropyl, PhCOCH2, etc.; R2 = Et, Pr, Me2CH, Bu, etc.; R3-R11 = H, CO2H, SH, SO3H, CONH2, (substituted) triazolyl, tetrazolyl, etc.; m = 1-4], effective angiotensin II antagonists useful in treating hypertension, congestive heart failure, etc., are prepared. Refluxing semicarbazide II (preparation given) with MeONa/MeOH in MePh gave 90% ester III (R = Me3C, R1 = H), which was treated with Me3COH/THF in DMF and then BuI to give 82% di-Bu derivative III (R = Me3C, R1 = Bu) (IV). Hydrolysis of IV with CF3CO2H in CHCl3 gave quant. acid III (R = H, R1 = Bu) which showed IC50 of 101 nM in angiotensin II binding activity. Also prepared and tested were 29 addnl. I.
 IT 139476-42-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as cardiovascular agent)
 RN 139476-43-0 CAPLUS
 CN 1H-1,2,4-Triazole-3-acetonitrile, 1-butyl-4,5-dihydro-5-oxo-u-propyl-4-[(2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)

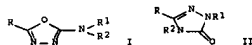


LS ANSWER 17 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1986:608833 CAPLUS Full-text
 DN 105:208833
 TI Oxidation of aldehyde semicarbazones with lead dioxide: application to the syntheses of 2-amino-1,3,4-oxadiazoles and 2,4-dihydro-1,2,4-triazol-3-ones

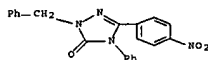
10529634

33 of 35

AU Thu Huong Nguyen; Milcent, Rene; Barbier, Geo
 CS Fac. Med., Univ. Paris, Paris, 75018, Fr.
 SO Journal of Heterocyclic Chemistry (1985), 22(5), 1383-8
 CODEN: JHTCAD; ISSN: 0022-152X
 DT Journal
 LA English
 OS CASREACT 105:208833
 GI



AB Treating 4,4-disubstituted semicarbazones of aromatic aldehydes
 RCH:NNHCONR1R2 (R = Ph, R1 = Me, R2 = H, Me; R = R2 = Ph; R = 4-MeOC6H4, 4-O2NC6H4, R1 = R2 = Me) with PbO2 in acidic media gave 2-amino-1,3,4-oxadiazoles I; the 2,4-disubstituted semicarbazones R3CH:NNH4CONHR5 (R3 = R4 = Ph, R5 = Me, Et, Pr, Bu, cyclohexyl, PhCH2, Ph, substituted Ph; R3 = substituted Ph, 4-pyridyl, R4 = Ph, R5 = Ph, substituted Ph) gave 2,4-dihydro-1,2,4-triazol-3-ones II, often in higher yields than the known methods.
 IT 104707-64-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 104707-64-4 CAPLUS
 CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-(4-nitrophenyl)-4-phenyl-2-(phenylmethyl)- (CA INDEX NAME)



L5 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 1972:526518 CAPLUS [Full-text](#)

DN 77:126518

OREF 77:20841a,20844a

TI Benzothiazole derivatives of 1,2,4-triazole

AU Russo, Filippo; Santagati, Maria; Pappalardo, Giovanni

CS Ist. Chim. Farm. Tossicol., Univ. Catania, Catania, Italy

SO Annali di Chimica (Rome, Italy) (1972), 62(5), 351-72

CODEN: ANCRAI; ISSN: 0003-4592

DT Journal

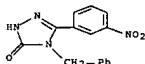
LA Italian

GI For diagram(s), see printed CA Issue.

AB 3-Amino-5-(2-benzothiazolyl)-1,2,4-triazoles (I, R = H, Me, Et, allyl) and the 3-methylthio analogs (II, R = alkyl, allyl, Ph) are prepared from 2-benzothiazolecarbohydrazide (III). III is treated with RNHC(SMe)NH and the products cyclized by NaOH to give I. The reaction products of III with RNCS are cyclized, and the products treated with MeI to give II. The

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=> log hold

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

106.94 290.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

ENTRY SESSION

CA SUBSCRIBER PRICE

-16.00 -16.00

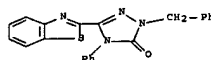
SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 16:50:27 ON 03 JAN 2009

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triazolinethione (IV) is obtained by the reaction of the hydrazide (V) with thiourea. About 70 compds. were prepared
 IT 37548-05-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 37548-05-3 CAPLUS
 CN 3H-1,2,4-Triazol-3-one, 5-(2-benzothiazolyl)-2,4-dihydro-4-phenyl-2-(phenylmethyl)- (CA INDEX NAME)



L5 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 1971:488541 CAPLUS [Full-text](#)

DN 75:88541

OREF 75:14021a,14024a

TI 3,4-Disubstituted 5-hydroxy-1,2,4-triazoles derived from 4-substituted semicarbazones

AU Husain, Syeda; Srinivasan, V. R.; Nath, T. G. Surendra

CS Dep. Chem., Osmania Univ., Hyderabad, India

SO Indian Journal of Chemistry (1971), 9(7), 642-6

CODEN: IJOCAP; ISSN: 0019-5103

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB 3-Aryl-4-alkyl-, 3,4-diaryl-, and 3-aryl-4-heterocyclic-5-hydroxy-1,2,4-triazoles, e.g. I, were prepared by the oxidative cyclization of the corresponding 4-substituted semicarbazones with K3Fe(CN)6 and alkali. Some 3-methyl-4-substituted-5-hydroxy-s-triazoles, when condensed with anisaldehyde, gave the corresponding styryl derivs., the trans-ethylenic configuration of which was established by their absorption in the 960-85 cm-1 region.

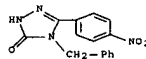
IT 33723-44-3P 33723-45-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 33723-44-3 CAPLUS

CN 4H-1,2,4-Triazol-3-ol, 4-benzyl-5-(p-nitrophenyl)- (8CI) (CA INDEX NAME)



RN 33723-45-4 CAPLUS

CN 4H-1,2,4-Triazol-3-ol, 4-benzyl-5-(m-nitrophenyl)- (8CI) (CA INDEX NAME)